

## Contents

1988 II, No. 1—6

### Recent Aspects of Fourier Transform Spectroscopy, Vol. 3

Proceedings of the 6th International Conference on Fourier Transform Spectroscopy, Vienna, August 24—28, 1987

G. Guelachvili, R. Kellner, G. Zerbi (eds.)

#### *Surfaces, Films, Catalysis*

FTIR Spectroscopy of Monomolecular Layers and Multilayers of Organic Molecules on Solid Substrates. <i>T. Arndt, C. Bubeck, A. J. Schouten, G. Wegner</i> (B 1.01) . . . . .	7
FTIR Characterization of Metal-Loaded Zeolites. <i>J. Baumann, R. Beer, G. Calzaferri</i> (B 1.03) . . . . .	11
An FT-IR Study of Adsorption of Sulfur Dioxide on Alpha- and Gamma-Alumina. <i>P. H. Berben, M. J. Kappers, J. W. Geus</i> (B 1.04) . . . . .	15
Overtone Surface Vibrational Spectroscopy of Zeolite-Encaged Molecules. <i>H. Böse, H. Förster</i> (B 1.05) . . . . .	19
FTIR Spectroscopy of Monolayers and Ultrathin Films Using Polarization Modulation. <i>T. Buffeteau, B. Desbat, J.-M. Turlet</i> (B 1.06) . . . . .	23
Surface and Adsorption Studies of High Surface Area Oxides. <i>E. Knözinger, P. Hoffmann, R. Echterhoff</i> (B 1.08) . . . . .	27
Fourier Transform Far-Infrared Studies on Transition Metal Ion-Exchanged Zeolites. <i>A. H. Förster, U. Witten</i> (B 1.09) . . . . .	35
Structure and Topography of Molecular Assemblies on Solid Substrates by Infrared Spectroscopy and Scanning Tunneling Microscopy. <i>V. M. Hallmark, A. Leone, S. Chiang, J. D. Swalen, J. F. Rabolt</i> (B 1.10) . . . . .	39

Enhanced Infrared ATR Spectra of Surface Layers of Polymers Using Metal Films. <i>M. Hirano, R. Nemori, Y. Nakao, H. Yamada</i> (B 1.11) . . . . .	43
Vibrational Spectra of Monolayer Islands on Single Crystal Faces. Island Size and Shape Effects on Infrared Frequencies, Intensities and Bandwidths. <i>S. F. Ippolitova, I. V. Kumpanenko, N. V. Chukhanov, S. G. Entelis</i> (B 1.12) . . . . .	47
Reflectance FTIR Investigations of the Reactions of Silanes on Silica Surfaces. <i>D. E. Leyden, R. S. S. Murthy, J. P. Blitz, J. B. Atwater, A. Rachetti</i> (B 1.13) . . . . .	53
FT-IR and FT-FIR Studies of Vanadium, Molybdenum and Tungsten Oxides Supported on Different Carriers. <i>F. Maugé, J.-P. Gallas, J.-C. Lavalley, G. Busca, G. Ramis, V. Lorenzelli</i> (B 1.14) . . . . .	57
Infrared Analysis of Thin Inorganic and Organic Films on Metals. <i>K. Molt, M. Egelkraut, K.-H. Gottwald</i> (B 1.15) . . . . .	63
Rearrangement of Langmuir-Blodgett Stearic Acid Films and Band Assignments in Deuterated Stearic Acid Monolayers. <i>R. L. Mowery, J. L. Dote</i> (B 1.16) . . . . .	69
Surface Oxidation of High-Surface-Area Silicon Carbide: FT-IR Studies. <i>P. Quintard, G. Ramis, M. Cauchetier, G. Busca, V. Lorenzelli</i> (B 1.17) . . . . .	75
Spectroscopic Infrared Ellipsometry by Means of FTS. <i>A. Röseler</i> (B 1.18) . . . . .	79
FTIR Spectroscopy of Ethyl Benzoate-Titanium Tetrachloride Complexes with Application to Supported Ziegler-Natta Catalysts. <i>E. Rytter, Ø. Nirisen, M. Ystnes, H. A. Øye</i> (B 1.19) . . . . .	85
Use of FTIR Spectroscopy in the Investigation of Catalytic Reactions in Zeolites—Possibilities and Limitations. <i>M. Schumann, H. Förster</i> (B 1.20) . . . . .	89
An FTIR Study of the Adsorption of Surfactants on Silica. <i>R. Sides, J. Yarwood, K. Fox</i> (B 1.22) . . . . .	93
Fourier Transform Infrared Investigations of Phosphate-Silicate Coatings on Iron. <i>A. Stoch, Cz. Palusziewicz, M. Handke</i> (B 1.23) . . . . .	97
Characterization of Alkali Exchanged ZSM5 by IR Spectroscopy. <i>G. Warecka, G. Rumplmayr, J. A. Lercher</i> (B 1.25) . . . . .	101
FTIR-Spectroscopy as a Highly Sensitive Technique to Study Adsorption and Desorption on Ionic Film and Single Crystal Surfaces. <i>J. Heidberg, E. Kampshoff, H. Stein, H. Weiss, M. War-skulat</i> (B 1.27) . . . . .	105

**Special Sampling (DRIFT, PAS)**

Resin Characterisation in Carbon Fibre Reinforced Prepregs Using Photoacoustic-FTIR. <i>J. M. Chalmers, J. Wilson</i> (B 2.02) . . . . .	109
"In-Situ" Drift Spectroscopy of Intracavity Chemistry of Carbonyl Complexes in Zeolites. <i>E. Denneulin, C. Brémard, C. Depecker, P. Legrand</i> (B 2.03) . . . . .	113
"In-Situ" Monitoring Activation and Reaction on Very Absorbing Catalytic Solid by DRIFT Spectrometer. <i>C. Depecker, P. Legrand, A. Sene, G. Wrobel</i> (B 2.04) . . . . .	119
Characterization of Chemically Modified Silica Gels by DRIFT Spectroscopy. <i>A. Fuchsgruber, W. Lindner, R. Dietl</i> (B 2.05) . . . . .	123
Rapid Quality Control of Solid Materials by Diffuse Reflectance FTIR Spectrometry. <i>P. M. Fredericks, K. J. Doolan</i> (B 2.06) . . . . .	127
Fourier Transform Infrared Photoacoustic Spectroscopy of Dental Calculus. <i>R.-Z. Hou, J.-G. Wu, R. D. Soloway, H. Guo, Y.-F. Zhang, Y.-C. Du, F. Liu, G.-X. Xu</i> (B 2.08) . . . . .	133
Diffuse Reflectance Spectroscopy—Important Developments. <i>M. Milošević</i> (B 2.12) . . . . .	137
Sampling Depth in Infrared Diffuse Reflection Spectroscopy of Undiluted Samples. <i>A. Otto, E.-H. Korte</i> (B 2.13) . . . . .	141
FTIR-PAS-Spectroscopic Study of Transparent Double-Layer Polymer Films. <i>J. Philippaerts, E. Vanderheyden, E. F. Vansant</i> (B 2.14) . . . . .	145
Quantitative Applications of Photoacoustic Spectroscopy in the Infrared. <i>R. J. Rosenthal, R. T. Carl, J. P. Beauchaine, M. P. Fuller</i> (B 2.15) . . . . .	149
Diffuse Reflectance Fourier Transform Infrared Spectroscopic Study of the Thermal Degradation of Barley Protein. <i>P. Savolahti</i> (B 2.16) . . . . .	155
In-Situ Measurement of Photochemical Changes of Solid Samples by Fourier Transform Infrared Photoacoustic Spectroscopy. <i>N. Teramae, S. Tanaka</i> (B 2.18) . . . . .	159
FTIR-PAS Analysis of Silica Gel Modified with Amines for the Treatment of Natural Gases Contaminated with Sulphur Compounds. <i>E. Vanderheyden, E. F. Vansant, J. Philippaerts</i> (B 2.19) . . . . .	163
Characterisation of Charcoals by DRIFT. <i>D. J. Wood</i> (B 2.20) . . . . .	167
FT-IR Photoacoustic Spectra of the Surface of Ru <sub>3</sub> (CO) <sub>12</sub> /Al <sub>2</sub> O <sub>3</sub> System. <i>Z.-H. Xu, I. S. Butler, J.-G. Wu, G.-X. Xu</i> (B 2.21) . . . . .	171
FT-IR/PAS Investigation of Solid Fuels and Catalysts. <i>T. Zerlia, A. Girelli</i> (B 2.22) . . . . .	175

***Coupled Techniques (GC-FTIR, LC-FTIR, SFC-FTIR)***

Scan-to-Scan Nonreproducibility in GC/FTIR: An Evaluation of Several Chromatogram Calculation Algorithms. <i>E. J. Darland</i> (B 3.01) . . . . .	179
The Continuous Infrared Spectroscopic Analysis of Reversed Phase Liquid Chromatography Separations. <i>J. J. Gagel, K. Biemann</i> (B 3.02) . . . . .	185
GC/FT-IR: A Unique Choice for Solvent Analysis. <i>K. Kempfert</i> (B 3.03) . . . . .	189
GC-FTIR and GC-MS in Odour Analysis of Essential Oils. <i>A. Nikiforov, L. Jirovetz, G. Buchbauer, V. Raverdino</i> (B 3.05) . . . . .	193
MAGIC-LC/FT-IR Spectrometry. <i>R. M. Robertson, J. A. de Haseth, R. F. Browner</i> (B 3.06) . . . . .	199
SFC/FT-IR: Supercritical Fluid Chromatography with Fourier Transform Infrared Detection. <i>R. C. Wieboldt, R. J. Rosenthal</i> (B 3.07) . . . . .	203

***FT-Raman***

A New Low Noise Detector for FT-Raman. <i>C. Tripp, H. Buijs</i> (B 4.02) . . . . .	209
FT-Raman Spectroscopy of Biological Molecules. <i>V. M. Hallmark, C. G. Zimba, J. D. Swalen, J. F. Rabolt</i> (B 4.03) . . . . .	215
Experimental Aspects of Fourier Transform Raman Spectroscopy. <i>J. F. Rabolt, C. G. Zimba, V. M. Hallmark, J. D. Swalen</i> (B 4.04) . . . . .	219
Fourier Transform Raman Spectroscopy in the Visible Region. <i>R. Savoie, P. Beauchesne, D. Lévesque</i> (B 4.05) . . . . .	223
Routine FT-Raman Spectroscopy with Modified Standard FT-IR Instrument. <i>B. Schrader, A. Simon</i> (B 4.06) . . . . .	227
Fourier Transform Raman Spectroscopy Using a Bench-Top Fourier Transform Infrared Spectrometer. <i>K. P. J. Williams, S. F. Parker, P. J. Hendra, A. J. Turner</i> (B 4.07) . . . . .	231
FT-Raman Studies of Langmuir-Blodgett Monolayer Components Containing Absorbing Chromophores. <i>C. G. Zimba, V. M. Hallmark, J. D. Swalen, J. F. Rabolt</i> (B 4.08) . . . . .	235

***Instrumentation, Double Modulation, Emission***

Matrix-Isolation-FTIR Spectroscopy with an Integrating Sphere. <i>E. Berger, D. W. T. Griffith, G. Schuster, S. R. Wilson</i> (B 5.03) . . . . .	239
Detector Quantum Efficiency: An Important Parameter for FT-IR Spectroscopy. <i>M. Birk, J. W. Brault</i> (B 5.04) . . . . .	243

Contents	VII
Some Observations on FTIR Emission Spectroscopy of Black Solid Samples. <i>J. M. Chalmers, M. W. Mackenzie, N. Poole</i> (B 5.06) . . . . .	249
A New Accessory for the Detection of Trace Components by FT-IR Spectroscopy. <i>B. Delahaye, P. Legrand, B. Sombret</i> (B 5.07) . . . . .	255
Bolometric Fourier Transform Spectroscopy. <i>J. E. Eldridge</i> (B 5.08) . . . . .	261
Zeeman-Modulation Fourier Transform Spectroscopy. <i>M. Elhanine, R. Farrenq, G. Guelachvili</i> (B 5.09) . . . . .	265
A New Compact Interferometer Design. <i>R. Goss, C. Wibbelmann</i> (B 5.10) . . . . .	271
FTIR Measurements of Optical Rotatory Dispersion and Circular Dichroism. <i>B. Jordanov, E.-H. Korte, B. Schrader</i> (B 5.12) . . . . .	275
Fourier Transform Vibrational Circular Dichroism and the Artifact Problem. <i>P. Malon, T. A. Keiderling</i> (B 5.14) . . . . .	279
A Millimetre-Wave Dispersive Fourier Transform Spectrometer. <i>R. J. Martin, K. Maries</i> (B 5.15) . . . . .	283
Channel Spectra Revisited. <i>D. A. Naylor, A. A. Schultz, S. E. Bougerolle, T. A. Clark</i> (B 5.16) . . . . .	289
A Large Optics Martin-Puplett Interferometer for Spectroscopy to Below 1.5 cm <sup>-1</sup> . <i>A. C. Nichol, F. L. Pratt, W. Hayes, J. R. Birch, R. Jefferies, G. O. Plumb</i> (B 5.17) . . . . .	295
A Rapid Scan Interferometer for Near Millimetre Wavelength Radiometry. <i>P. G. Quincey, A. Mukherjee, J. S. Elder, E. A. Baker, D. G. Moss, J. R. Birch</i> (B 5.18) . . . . .	299
Performance Data of the Double Pendulum Interferometer. <i>H. Rippel, R. Jaacks</i> (B 5.19) . . . . .	303
Band Distortions in Emission and Specular Reflection FTIR Spectroscopy. <i>E. Rytter, M.-A. Einarssrud</i> (B 5.20) . . . . .	307
FT Transmission Spectroscopy in the Visible and Ultraviolet Spectral Ranges. <i>A. Simon, L. Wunsch, G. Zachmann</i> (B 5.22) . . . . .	311
An Investigation of High Temperature Phonon Anharmonicity of KCl by the FT-IR Emission Technique. <i>H. Tanaka, K. Hisano</i> (B 5.24) .	315
Pathlength Alteration in an Interferometer by Rotation of a Retro-reflector. <i>V. Tank</i> (B 5.25) . . . . .	319
Signal-to-Noise Characteristics of Photodiode Array Fourier Transform Spectrometers. <i>R. A. Van Tassel, W. K. Wong</i> (B 5.27) . .	323

Vibrational Circular Dichroism of Polypeptides and Proteins. <i>S. C. Yasui, T. A. Keiderling</i> (B 5.29) . . . . .	325
A Fourier Transform Visible Spectrometer. <i>Z.-L. Zhang, P. Zheng, Z. Lin</i> (B 5.30) . . . . .	329

#### **FTIR-Condensed Matter**

FT-Far-Infrared Spectroscopic Studies of Solute-Solvent Interactions and Molecular Dynamics in Solutions of Methanol, <i>N</i> -Methyl Formamide and <i>N,N</i> -Dimethyl Formamide. <i>R. Buchner, J. Yarwood</i> (B 6.01) . . . . .	335
Far Infrared Spectra of Solid Molecular Nitrogen. <i>G. Guelachvili, K. N. Rao, R. H. Tipping, B. P. Winnewisser, M. Winnewisser</i> (B 6.02) . . . . .	339
Far Infrared Reflectivity of Narrow Band Materials. <i>F. Marabelli, L. Degiorgi, P. Wachter</i> (B 6.03) . . . . .	345
Far Infrared Spectra of Liquid and Solid Benzene. <i>R. C. F. Mrozek, W. F. Sherman, G. R. Wilkinson</i> (B 6.04) . . . . .	349
IR-Active Lattice Modes of $\alpha$ -Glycine and Deutero- $\alpha$ -Glycine. <i>R. Ramnarine, W. F. Sherman, C. J. Chunnillall</i> (B 6.05) . . . . .	353
Application of FTIR Spectroscopy in the Study of Lattice Vibration for Mixed Crystals. <i>X.-C. Shen, H.-J. Ye, W. Lu</i> (B 6.06) . . . . .	357
Far Infrared Transmission Measurements of the Lattice Response of GaAs at 300 and 100 K. <i>A. K. Wan Abdullah, T. J. Parker</i> (B 6.07) . . . . .	361
FT Far-IR Investigation of Rare Earth Nitrates in Non-Aqueous Solution. <i>J.-G. Wu, N. Shi, H.-C. Gao, T.-Z. Jin, G.-X. Xu</i> (B 6.09) . . . . .	365
FT Far IR Studies of $\text{YBa}_2\text{Cu}_3\text{O}_x$ and Ln-Ba-Cu-O Superconductor Systems. <i>H.-Z. Liu, Z.-H. Xu, S.-F. Weng, W.-J. Zhou, H. Guo, Y.-Z. Lin, J.-F. Wang, F.-A. Liu, D.-F. Xu, J.-G. Wu, G.-X. Xu</i> (B 6.10) . . . . .	369

#### **Theoretical—Part 2**

FT-IR Determinations in Charge-Transfer Interactions Between Phenylhydrazones and Organic Acceptors. <i>P. Bruni, L. Cardellini, G. Tosi</i> (B 7.02) . . . . .	373
Complexes Between HCl and Proton Acceptors in Gas and Low Temperature Argon Matrices. <i>J. K. Corbett, W. O. George, R. Lewis</i> (B 7.03) . . . . .	375
FTIR Reflection Spectra and Structure of Molten Chloroaluminates Containing Alkaline Earth Chlorides or Oxides. <i>M.-A. Einarsson, E. Rytter</i> (B 7.04) . . . . .	381

Hydrogen Bond Lengths in Aqueous Hydroxylammonium Nitrate as a Function of Concentration, Temperature and Pressure. <i>R. A. Fifer</i> (B 7.05) . . . . .	385
IR-Dichroism of Metal Dithiocarbamate Single Crystals by Attenuated Total Reflectance Spectroscopy. <i>N. Tredafilova, G. St. Nikolov, H. Mikosch, G. Bauer, R. Kellner</i> (B 7.11) . . . . .	391
Vibrational Analysis and FTIR Spectra of Seven Isotopic Congeners of Ethyl Benzoate Including $^{18}\text{O}$ Carbonyl and Ether Labelled Esters. <i>M. Ystenes, E. Rytter</i> (B 7.12) . . . . .	395

#### *High Resolution and Atmospheric Studies*

How High-Resolution FTS Can Help in Assigning Pumped Laser Lines and Vice-Versa. <i>T. Al Adlouni, G. Graner</i> (B 8.01) . . . . .	399
High Resolution Fourier Spectroscopy of Nitrous Oxide at Elevated Temperatures. <i>M. P. Esplin, W. M. Barowy, R. J. Huppi, G. A. Vanasse</i> (B 8.02) . . . . .	403
Quantification of Several Atmospheric Gases from High Resolution Infrared Solar Spectra Obtained at the South Pole in 1980 and 1986. <i>A. Goldman, F. J. Murcray, F. H. Murcray, D. G. Murcray, C. P. Rinsland</i> (B 8.06) . . . . .	409
High Resolution FT-IR Spectrum of Tricarbon Disulfide, S <sub>CCCS</sub> . <i>F. Holland, M. Winnewisser, J. W. C. Johns</i> (B 8.07) . . . . .	417
A Radiometric Fourier Transform Spectrometer for the Measurement of Downwelling Atmospheric Emission. <i>D. D. LaPorte, J. D. Carpenter, H. E. Revercomb</i> (B 8.09) . . . . .	421
Rotational Analysis of Nitrosyl Chloride. <i>J. K. McDonald, V. F. Kalasinsky, T. J. Geyer, J. R. Durig</i> (B 8.12) . . . . .	429
Observation of Upwelling Radiation by SCRIBE. <i>F. J. Murcray, F. H. Murcray, D. G. Murcray, J. J. Kosters, W. J. Williams, G. A. Vanasse</i> (B 8.13) . . . . .	433
High-Altitude Aircraft Measurements of Upwelling IR Radiance: Prelude to FTIR from Geosynchronous Satellite. <i>H. E. Revercomb, D. D. LaPorte, W. L. Smith, H. Buijs, D. G. Murcray, F. J. Murcray, L. A. Sromovsky</i> (B 8.15) . . . . .	439
High Resolution FTS of Atoms and Molecules in the Ultra-Violet. <i>A. P. Thorne, R. C. M. Learner</i> (B 8.16) . . . . .	445

#### *News Section*

Announcement: 7th International Conference on Fourier Transform Spectroscopy, George Mason University, Fairfax, VA, USA, June 19–23, 1989 . . . . .	449
-----------------------------------------------------------------------------------------------------------------------------------------------------	-----

Announcement: 1989 European Plasma Winter Conference on Spec-	
trochemistry, Reutte/Tyrol, Austria, January 8—14, 1989 . . . . .	452
Conference Calendar . . . . .	454

Impressum siehe S. 456

Abstracted/Index in: Current Contents, SCI, ASCA, Analytical Abstracts, Biosis, Chemical Abstracts

